Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*S*)-*N*-(1-Phenylethylpiperidin-1-ium-3-ylmethyl)-*N*-phenylpropionamide trifluoroacetate

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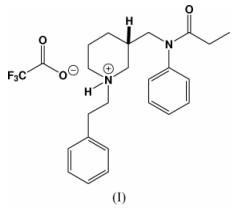
Received 30 June 2003
Accepted 16 July 2003
Online 30 August 2003

The synthesis and crystal structure of the title compound, $C_{25}H_{31}F_3N_2O_3$, are reported.



(I)

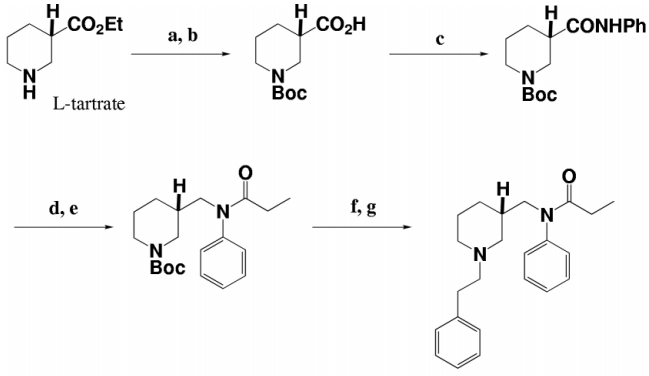
Key indicators

Single-crystal X-ray study
T = 213 K
Mean σ(C–C) = 0.004 Å
Disorder in solvent or counterion
R factor = 0.047
wR factor = 0.125
Data-to-parameter ratio = 10.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Experimental

The title compound was synthesized from ethyl (*S*)-nipecotate L-tartrate (see reaction Scheme). Crystals were grown from an ethyl acetate solution.



(**a**) Boc_2O, NEt_3, Dioxan-H_2O, r.t., 4h. (**b**) LiOH, H_2O, 0 °C. (**c**) $PhNH_2$, DCC, CH_2Cl_2, r.t. (**d**) Borane, THF, reflux, 2h. (**e**) EtCOCl, $^iPr_2NEt$, CH_2Cl_2, r.t. (**f**) TFA, CH_2Cl_2, 0 °C. (**g**) $PhCH_2CH_2Br$, K_2CO_3, CH_3CN, 65 °C.
Boc: tert-BuOCO-; DCC; 1,3-Dicyclohexylcarbodiimide.

Crystal data

$C_{23}H_{31}N_2O^+\cdot C_2F_3O_2^-$
M_r = 464.52
Orthorhombic, $P2_12_12_1$
a = 10.1973 (7) Å
b = 10.8295 (7) Å
c = 21.9100 (10) Å
V = 2419.6 (3) Å^3
Z = 4
D_x = 1.275 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 648 reflections
θ = 3.0–28.7°
μ = 0.10 mm^{-1}
T = 213 (2) K
Plate, colorless
0.25 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
ω scans
15 557 measured reflections
3332 independent reflections
3113 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 28.3°
h = −13 → 13
k = −14 → 9
l = −28 → 26

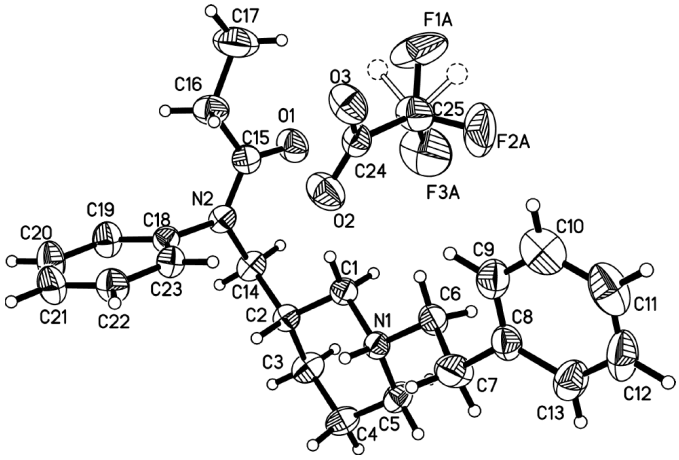


Figure 1
Displacement ellipsoid plot (50% probability level) of the title compound.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.125$
$S = 1.10$
3332 reflections
321 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0653P)^2 + 0.52P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3^{i}	0.91 (3)	1.82 (3)	2.722 (2)	178 (2)

Symmetry code: (i) $1-x, \frac{1}{2}+y, \frac{1}{2}-z$.

Carbon-bound H atoms were placed in idealized positions and refined as riding, with C—H = 0.94 Å (0.98 Å for methyl H atoms). Nitrogen-bound H atoms were refined freely. Friedel pairs were merged for the final refinement since no atoms heavier than F are present and the absolute configuration was known.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1998); software used to prepare material for publication: *SHELXL*97.

References

Bruker (1997). *SMART*. Version 5.054. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SAINT*. Version 6.01. Bruker AXS Inc., Madison, Wisconsin, USA.
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Sheldrick, G. M.(1997). *SHELXL*97. University of Göttingen, Germany.
Sheldrick, G. M. (1998). *SHELXTL*. Version 5.10. Bruker AXS Inc, Madison, Wisconsin, USA.

supporting information

Acta Cryst. (2003). E**59**, o1398–o1399 [doi:10.1107/S1600536803015654]

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S1. Comment

NO COMMENT

S2. Experimental

The title compound was synthesized from ethyl (S)-nipecotate *L*-tartrate (see reaction Scheme). Crystals were grown from an ethyl acetate solution.

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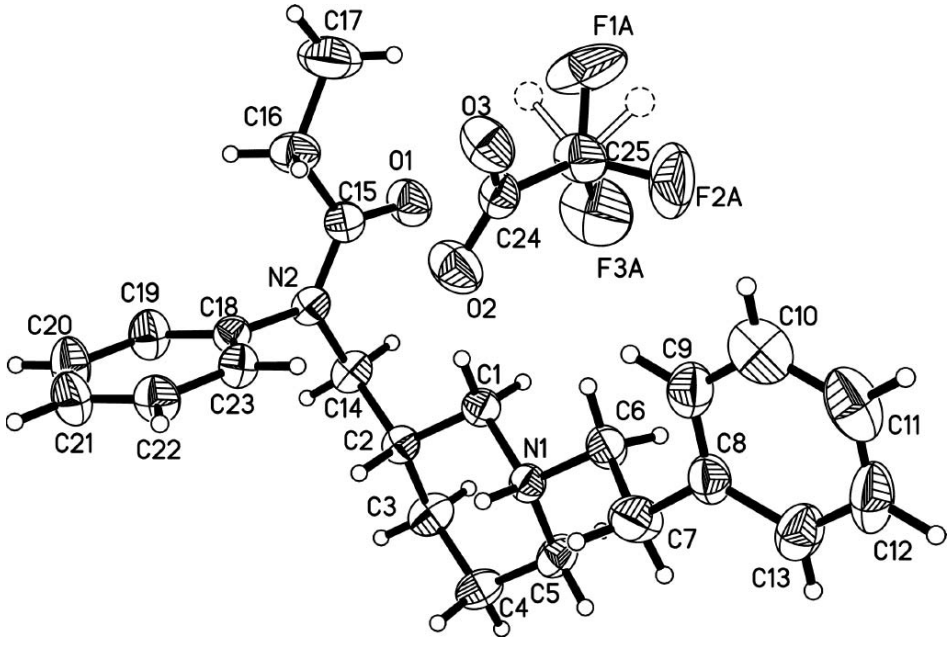
Carbon-bound H atoms were placed in idealized positions and refined as a riding model, with C—H = 0.94 Å (0.98 Å for methyl H atoms). Nitrogen-bound H atoms was freely refined. Friedel pairs were merged for the final refinement since no atoms heavier than Si are present and the absolute configuration was known.



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Displacement ellipsoid plot (50% probability) of the title compound.

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Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 648 reflections
$\theta = 3.0$–$28.7°$
$\mu = 0.10$ mm^{-1}
$T = 213$ K
Needle, colorless
0.25 × 0.20 × 0.10 mm

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Bruker CCD diffractometer
Radiation source: normal-focus sealed tube
Graphite monochromator
Detector resolution: 8.3 pixels mm^{-1}
ω scans
15557 measured reflections
3332 independent reflections
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$R_{int} = 0.055$
$\theta_{max} = 28.3°$, $\theta_{min} = 1.9°$
$h = -13 \rightarrow 13$
$k = -14 \rightarrow 9$
$l = -28 \rightarrow 26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.125$
$S = 1.10$
3332 reflections
321 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0653P)^2 + 0.52P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}

Special details

Experimental. Data was collected using a Bruker *SMART* CCD (charge coupled device) based diffractometer equipped with an LT-2 low-temperature apparatus operating at 213 K. A suitable crystal was chosen and mounted on a glass fiber using grease. Data were measured using omega scans of 0.3° per frame for 30 s, such that a hemisphere was collected. A total of 1271 frames were collected with a final resolution of 0.75 Å. The first 50 frames were recollected at the end of data collection to monitor for decay. Cell parameters were retrieved using *SMART* software and refined using *SAINT* on all observed reflections. Data reduction was performed using the *SAINT* software which corrects for Lp and decay. Absorption corrections were applied using *SADABS* based on Blessing, (1995). The structures are solved by the direct method using the *SHELX90* program and refined by least squares method on F2 *SHELXL93*, incorporated in *SHELXTL* V5.1.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.77365 (19)	0.6452 (2)	0.25998 (9)	0.0335 (4)	
H1A	0.8599	0.6417	0.2404	0.040*	
H1B	0.7441	0.5604	0.2675	0.040*	
O1	0.97375 (17)	0.42215 (18)	0.32919 (8)	0.0510 (4)	
N1	0.67772 (16)	0.71023 (16)	0.21882 (7)	0.0311 (3)	
H1	0.602 (3)	0.704 (2)	0.2403 (11)	0.029 (6)*	
N2	0.81872 (16)	0.52443 (16)	0.38306 (8)	0.0334 (4)	
C2	0.78372 (19)	0.71502 (19)	0.32052 (9)	0.0322 (4)	
H2A	0.6947	0.7199	0.3384	0.039*	
C3	0.8317 (2)	0.8468 (2)	0.30927 (11)	0.0436 (5)	
H3A	0.8347	0.8919	0.3480	0.052*	
H3B	0.9206	0.8447	0.2923	0.052*	
C4	0.7400 (3)	0.9130 (2)	0.26492 (11)	0.0449 (5)	
H4A	0.6546	0.9253	0.2845	0.054*	
H4B	0.7762	0.9946	0.2553	0.054*	
C5	0.7211 (2)	0.8410 (2)	0.20607 (10)	0.0411 (5)	
H5A	0.6551	0.8824	0.1808	0.049*	
H5B	0.8037	0.8396	0.1832	0.049*	
C6	0.6530 (2)	0.6370 (2)	0.16163 (9)	0.0395 (5)	
H6A	0.6490	0.5490	0.1717	0.047*	
H6B	0.7257	0.6495	0.1331	0.047*	
C7	0.5250 (3)	0.6761 (3)	0.13135 (13)	0.0581 (7)	
H7A	0.4559	0.6789	0.1624	0.070*	
H7B	0.5355	0.7597	0.1150	0.070*	
C8	0.4811 (2)	0.5912 (2)	0.08004 (10)	0.0419 (5)	
C9	0.4668 (3)	0.4647 (3)	0.08934 (11)	0.0493 (6)	
H9A	0.4886	0.4305	0.1275	0.059*	
C10	0.4211 (3)	0.3888 (3)	0.04330 (15)	0.0631 (8)	
H10A	0.4127	0.3035	0.0503	0.076*	
C11	0.3881 (3)	0.4365 (4)	−0.01218 (14)	0.0652 (9)	
H11A	0.3565	0.3845	−0.0433	0.078*	
C12	0.4016 (3)	0.5629 (4)	−0.02249 (11)	0.0626 (8)	
H12A	0.3790	0.5962	−0.0607	0.075*	
C13	0.4479 (2)	0.6395 (3)	0.02312 (11)	0.0516 (6)	
H13A	0.4570	0.7246	0.0157	0.062*	
C14	0.8715 (2)	0.6460 (2)	0.36570 (10)	0.0372 (4)	
H14A	0.9584	0.6348	0.3474	0.045*	
H14B	0.8821	0.6963	0.4025	0.045*	
C15	0.8777 (2)	0.4190 (2)	0.36282 (10)	0.0367 (4)	
C16	0.8188 (2)	0.2982 (2)	0.38471 (13)	0.0468 (5)	
H16A	0.8115	0.3006	0.4293	0.056*	
H16B	0.7301	0.2903	0.3680	0.056*	
C17	0.8974 (4)	0.1863 (3)	0.3667 (2)	0.0798 (11)	
H17A	0.8546	0.1125	0.3819	0.120*	
H17B	0.9848	0.1922	0.3839	0.120*	

H17C	0.9034	0.1821	0.3225	0.120*	
C18	0.70467 (19)	0.52458 (19)	0.42202 (9)	0.0320 (4)	
C19	0.7195 (2)	0.5384 (3)	0.48496 (10)	0.0453 (5)	
H19A	0.8037	0.5449	0.5021	0.054*	
C20	0.6095 (3)	0.5426 (3)	0.52228 (11)	0.0543 (7)	
H20A	0.6194	0.5510	0.5647	0.065*	
C21	0.4846 (3)	0.5345 (3)	0.49701 (11)	0.0503 (6)	
H21A	0.4102	0.5380	0.5223	0.060*	
C22	0.4704 (2)	0.5214 (2)	0.43472 (11)	0.0427 (5)	
H22A	0.3860	0.5161	0.4177	0.051*	
C23	0.5796 (2)	0.5161 (2)	0.39692 (9)	0.0353 (4)	
H23A	0.5690	0.5068	0.3545	0.042*	
C24	0.6211 (2)	0.2773 (2)	0.22002 (10)	0.0358 (4)	
C25	0.7464 (3)	0.2675 (3)	0.18029 (14)	0.0545 (7)	
O2	0.6075 (2)	0.37242 (18)	0.24934 (10)	0.0580 (5)	
O3	0.54885 (17)	0.18503 (18)	0.21666 (9)	0.0510 (4)	
F1A	0.8041 (6)	0.1650 (5)	0.1804 (4)	0.124 (4)	0.652 (10)
F2A	0.7053 (5)	0.2798 (5)	0.11853 (14)	0.0872 (14)	0.652 (10)
F3A	0.8201 (2)	0.3675 (2)	0.17958 (13)	0.0973 (8)	
F1B	0.8463 (5)	0.2175 (9)	0.2244 (4)	0.083 (3)	0.348 (10)
F2B	0.7531 (9)	0.1915 (18)	0.1416 (7)	0.153 (9)	0.348 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0266 (9)	0.0381 (10)	0.0357 (9)	0.0026 (8)	0.0002 (7)	0.0028 (8)
O1	0.0375 (8)	0.0587 (10)	0.0567 (9)	0.0022 (8)	0.0122 (8)	−0.0017 (9)
N1	0.0254 (7)	0.0369 (8)	0.0308 (7)	0.0013 (7)	0.0025 (6)	0.0026 (7)
N2	0.0262 (7)	0.0364 (8)	0.0377 (8)	−0.0022 (7)	−0.0009 (7)	0.0061 (7)
C2	0.0274 (8)	0.0336 (9)	0.0355 (9)	−0.0031 (8)	0.0005 (8)	0.0027 (8)
C3	0.0412 (11)	0.0394 (11)	0.0503 (12)	−0.0092 (10)	−0.0070 (10)	0.0052 (10)
C4	0.0485 (12)	0.0329 (10)	0.0534 (12)	−0.0045 (10)	−0.0046 (10)	0.0085 (9)
C5	0.0392 (11)	0.0425 (11)	0.0416 (11)	−0.0045 (10)	0.0020 (9)	0.0124 (9)
C6	0.0371 (10)	0.0475 (11)	0.0338 (9)	0.0066 (10)	−0.0007 (8)	−0.0037 (9)
C7	0.0633 (16)	0.0618 (16)	0.0492 (13)	0.0230 (14)	−0.0232 (12)	−0.0141 (13)
C8	0.0370 (10)	0.0554 (13)	0.0333 (9)	0.0064 (11)	−0.0011 (8)	−0.0030 (9)
C9	0.0480 (13)	0.0601 (14)	0.0397 (11)	0.0018 (12)	0.0041 (10)	0.0037 (11)
C10	0.0493 (14)	0.0662 (18)	0.0739 (18)	−0.0105 (14)	0.0034 (14)	−0.0128 (15)
C11	0.0412 (13)	0.098 (3)	0.0567 (16)	−0.0039 (15)	−0.0048 (12)	−0.0291 (16)
C12	0.0441 (13)	0.111 (3)	0.0324 (10)	0.0085 (16)	−0.0036 (10)	0.0020 (13)
C13	0.0424 (12)	0.0692 (16)	0.0433 (12)	0.0031 (12)	−0.0041 (10)	0.0091 (12)
C14	0.0300 (9)	0.0406 (10)	0.0409 (10)	−0.0082 (9)	−0.0054 (8)	0.0056 (9)
C15	0.0308 (9)	0.0420 (10)	0.0373 (9)	0.0017 (9)	−0.0035 (8)	0.0004 (9)
C16	0.0415 (12)	0.0371 (11)	0.0618 (14)	−0.0013 (10)	0.0018 (11)	−0.0003 (10)
C17	0.094 (3)	0.0415 (14)	0.103 (3)	0.0113 (16)	0.014 (2)	−0.0055 (16)
C18	0.0291 (9)	0.0333 (9)	0.0336 (9)	0.0007 (8)	−0.0003 (7)	0.0026 (8)
C19	0.0371 (11)	0.0625 (14)	0.0363 (10)	−0.0018 (11)	−0.0054 (9)	−0.0006 (10)
C20	0.0534 (14)	0.0777 (18)	0.0318 (10)	−0.0022 (14)	0.0012 (10)	−0.0048 (11)

C21	0.0423 (12)	0.0648 (15)	0.0438 (11)	0.0002 (12)	0.0125 (10)	−0.0025 (12)
C22	0.0296 (9)	0.0508 (12)	0.0478 (11)	−0.0013 (10)	0.0011 (9)	−0.0001 (11)
C23	0.0319 (9)	0.0413 (10)	0.0326 (9)	−0.0033 (9)	−0.0025 (8)	0.0007 (8)
C24	0.0268 (9)	0.0460 (11)	0.0348 (9)	0.0022 (9)	0.0032 (8)	0.0052 (9)
C25	0.0395 (12)	0.0518 (14)	0.0722 (17)	0.0014 (11)	0.0238 (12)	0.0040 (13)
O2	0.0544 (11)	0.0513 (10)	0.0683 (11)	−0.0046 (9)	0.0206 (10)	−0.0104 (9)
O3	0.0371 (8)	0.0556 (10)	0.0602 (10)	−0.0079 (8)	0.0126 (8)	−0.0119 (9)
F1A	0.096 (4)	0.091 (4)	0.184 (8)	0.065 (4)	0.098 (5)	0.083 (5)
F2A	0.081 (3)	0.130 (3)	0.0511 (16)	0.015 (2)	0.0311 (15)	0.017 (2)
F3A	0.0594 (11)	0.0963 (15)	0.136 (2)	−0.0175 (12)	0.0426 (13)	0.0020 (15)
F1B	0.036 (2)	0.127 (6)	0.086 (5)	0.023 (3)	0.006 (3)	0.009 (5)
F2B	0.070 (6)	0.26 (2)	0.131 (9)	−0.056 (9)	0.048 (6)	−0.155 (12)

Geometric parameters (Å, º)

C1—N1	1.505 (2)	C11—C12	1.395 (5)
C1—C2	1.530 (3)	C11—H11A	0.9400
C1—H1A	0.9800	C12—C13	1.382 (4)
C1—H1B	0.9800	C12—H12A	0.9400
O1—C15	1.226 (3)	C13—H13A	0.9400
N1—C6	1.504 (3)	C14—H14A	0.9800
N1—C5	1.510 (3)	C14—H14B	0.9800
N1—H1	0.91 (3)	C15—C16	1.517 (3)
N2—C15	1.364 (3)	C16—C17	1.506 (4)
N2—C18	1.443 (2)	C16—H16A	0.9800
N2—C14	1.472 (3)	C16—H16B	0.9800
C2—C3	1.529 (3)	C17—H17A	0.9700
C2—C14	1.530 (3)	C17—H17B	0.9700
C2—H2A	0.9900	C17—H17C	0.9700
C3—C4	1.528 (3)	C18—C23	1.392 (3)
C3—H3A	0.9800	C18—C19	1.395 (3)
C3—H3B	0.9800	C19—C20	1.389 (4)
C4—C5	1.519 (3)	C19—H19A	0.9400
C4—H4A	0.9800	C20—C21	1.391 (4)
C4—H4B	0.9800	C20—H20A	0.9400
C5—H5A	0.9800	C21—C22	1.380 (3)
C5—H5B	0.9800	C21—H21A	0.9400
C6—C7	1.524 (3)	C22—C23	1.389 (3)
C6—H6A	0.9800	C22—H22A	0.9400
C6—H6B	0.9800	C23—H23A	0.9400
C7—C8	1.520 (3)	C24—O2	1.222 (3)
C7—H7A	0.9800	C24—O3	1.244 (3)
C7—H7B	0.9800	C24—C25	1.550 (3)
C8—C9	1.393 (4)	C25—F2B	1.184 (8)
C8—C13	1.394 (3)	C25—F1A	1.256 (4)
C9—C10	1.382 (4)	C25—F3A	1.318 (3)
C9—H9A	0.9400	C25—F2A	1.423 (5)
C10—C11	1.363 (5)	C25—F1B	1.506 (7)

C10—H10A	0.9400

N1—C1—C2	109.37 (16)	C13—C12—C11	120.4 (3)
N1—C1—H1A	109.8	C13—C12—H12A	119.8
C2—C1—H1A	109.8	C11—C12—H12A	119.8
N1—C1—H1B	109.8	C12—C13—C8	120.3 (3)
C2—C1—H1B	109.8	C12—C13—H13A	119.8
H1A—C1—H1B	108.2	C8—C13—H13A	119.8
C6—N1—C1	111.20 (16)	N2—C14—C2	112.98 (16)
C6—N1—C5	112.91 (16)	N2—C14—H14A	109.0
C1—N1—C5	111.06 (16)	C2—C14—H14A	109.0
C6—N1—H1	104.6 (15)	N2—C14—H14B	109.0
C1—N1—H1	101.8 (15)	C2—C14—H14B	109.0
C5—N1—H1	114.6 (16)	H14A—C14—H14B	107.8
C15—N2—C18	123.27 (17)	O1—C15—N2	121.6 (2)
C15—N2—C14	120.20 (17)	O1—C15—C16	122.0 (2)
C18—N2—C14	116.53 (17)	N2—C15—C16	116.37 (18)
C3—C2—C14	111.92 (17)	C17—C16—C15	113.6 (2)
C3—C2—C1	110.06 (17)	C17—C16—H16A	108.8
C14—C2—C1	111.01 (17)	C15—C16—H16A	108.8
C3—C2—H2A	107.9	C17—C16—H16B	108.8
C14—C2—H2A	107.9	C15—C16—H16B	108.8
C1—C2—H2A	107.9	H16A—C16—H16B	107.7
C4—C3—C2	110.17 (19)	C16—C17—H17A	109.5
C4—C3—H3A	109.6	C16—C17—H17B	109.5
C2—C3—H3A	109.6	H17A—C17—H17B	109.5
C4—C3—H3B	109.6	C16—C17—H17C	109.5
C2—C3—H3B	109.6	H17A—C17—H17C	109.5
H3A—C3—H3B	108.1	H17B—C17—H17C	109.5
C5—C4—C3	112.1 (2)	C23—C18—C19	119.77 (19)
C5—C4—H4A	109.2	C23—C18—N2	120.32 (17)
C3—C4—H4A	109.2	C19—C18—N2	119.86 (18)
C5—C4—H4B	109.2	C20—C19—C18	119.9 (2)
C3—C4—H4B	109.2	C20—C19—H19A	120.1
H4A—C4—H4B	107.9	C18—C19—H19A	120.1
N1—C5—C4	111.21 (17)	C19—C20—C21	120.2 (2)
N1—C5—H5A	109.4	C19—C20—H20A	119.9
C4—C5—H5A	109.4	C21—C20—H20A	119.9
N1—C5—H5B	109.4	C22—C21—C20	119.7 (2)
C4—C5—H5B	109.4	C22—C21—H21A	120.1
H5A—C5—H5B	108.0	C20—C21—H21A	120.1
N1—C6—C7	111.12 (18)	C21—C22—C23	120.7 (2)
N1—C6—H6A	109.4	C21—C22—H22A	119.7
C7—C6—H6A	109.4	C23—C22—H22A	119.7
N1—C6—H6B	109.4	C22—C23—C18	119.75 (18)
C7—C6—H6B	109.4	C22—C23—H23A	120.1
H6A—C6—H6B	108.0	C18—C23—H23A	120.1
C8—C7—C6	114.0 (2)	O2—C24—O3	129.9 (2)

C8—C7—H7A	108.8	O2—C24—C25	116.5 (2)
C6—C7—H7A	108.8	O3—C24—C25	113.6 (2)
C8—C7—H7B	108.8	F2B—C25—F1A	50.2 (8)
C6—C7—H7B	108.8	F2B—C25—F3A	122.0 (7)
H7A—C7—H7B	107.7	F1A—C25—F3A	117.3 (4)
C9—C8—C13	118.3 (2)	F2B—C25—F2A	53.2 (11)
C9—C8—C7	121.2 (2)	F1A—C25—F2A	102.8 (5)
C13—C8—C7	120.4 (2)	F3A—C25—F2A	94.6 (3)
C10—C9—C8	120.9 (3)	F2B—C25—F1B	99.8 (9)
C10—C9—H9A	119.6	F1A—C25—F1B	50.5 (4)
C8—C9—H9A	119.6	F3A—C25—F1B	85.3 (4)
C11—C10—C9	120.6 (3)	F2A—C25—F1B	147.6 (4)
C11—C10—H10A	119.7	F2B—C25—C24	119.8 (5)
C9—C10—H10A	119.7	F1A—C25—C24	116.5 (3)
C10—C11—C12	119.5 (3)	F3A—C25—C24	114.9 (2)
C10—C11—H11A	120.3	F2A—C25—C24	106.6 (3)
C12—C11—H11A	120.3	F1B—C25—C24	102.8 (3)

C2—C1—N1—C6	−173.50 (16)	C14—N2—C15—O1	−1.3 (3)
C2—C1—N1—C5	59.9 (2)	C18—N2—C15—C16	−1.4 (3)
N1—C1—C2—C3	−60.3 (2)	C14—N2—C15—C16	178.2 (2)
N1—C1—C2—C14	175.23 (16)	O1—C15—C16—C17	6.0 (4)
C14—C2—C3—C4	−178.9 (2)	N2—C15—C16—C17	−173.4 (3)
C1—C2—C3—C4	57.1 (2)	C15—N2—C18—C23	−85.5 (3)
C2—C3—C4—C5	−53.9 (3)	C14—N2—C18—C23	94.9 (2)
C6—N1—C5—C4	177.84 (19)	C15—N2—C18—C19	97.2 (3)
C1—N1—C5—C4	−56.5 (2)	C14—N2—C18—C19	−82.4 (3)
C3—C4—C5—N1	53.4 (3)	C23—C18—C19—C20	0.6 (4)
C1—N1—C6—C7	159.9 (2)	N2—C18—C19—C20	177.9 (2)
C5—N1—C6—C7	−74.5 (2)	C18—C19—C20—C21	−0.8 (4)
N1—C6—C7—C8	−169.6 (2)	C19—C20—C21—C22	0.4 (5)
C6—C7—C8—C9	54.2 (4)	C20—C21—C22—C23	0.1 (4)
C6—C7—C8—C13	−129.0 (3)	C21—C22—C23—C18	−0.3 (4)
C13—C8—C9—C10	0.2 (4)	C19—C18—C23—C22	0.0 (3)
C7—C8—C9—C10	177.0 (3)	N2—C18—C23—C22	−177.4 (2)
C8—C9—C10—C11	−0.5 (4)	O2—C24—C25—F2B	−164.3 (14)
C9—C10—C11—C12	0.4 (4)	O3—C24—C25—F2B	15.5 (14)
C10—C11—C12—C13	−0.1 (5)	O2—C24—C25—F1A	138.3 (6)
C11—C12—C13—C8	−0.3 (4)	O3—C24—C25—F1A	−41.9 (7)
C9—C8—C13—C12	0.2 (4)	O2—C24—C25—F3A	−4.4 (4)
C7—C8—C13—C12	−176.6 (3)	O3—C24—C25—F3A	175.4 (3)
C15—N2—C14—C2	109.1 (2)	O2—C24—C25—F2A	−107.7 (3)
C18—N2—C14—C2	−71.3 (2)	O3—C24—C25—F2A	72.1 (3)
C3—C2—C14—N2	173.01 (18)	O2—C24—C25—F1B	86.3 (5)
C1—C2—C14—N2	−63.6 (2)	O3—C24—C25—F1B	−93.9 (5)
C18—N2—C15—O1	179.20 (19)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O3^{i}	0.91 (3)	1.82 (3)	2.722 (2)	178 (2)

Symmetry code: (i) −*x*+1, *y*+1/2, −*z*+1/2.